Author Search

```
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FILE COVERS 1907 - 24 Aug 2007  VOL 147 ISS 10
FILE LAST UPDATED: 23 Aug 2007  (20070823/ED)

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=> D QUE L8
L1                STR
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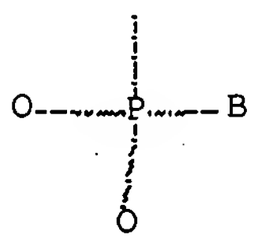


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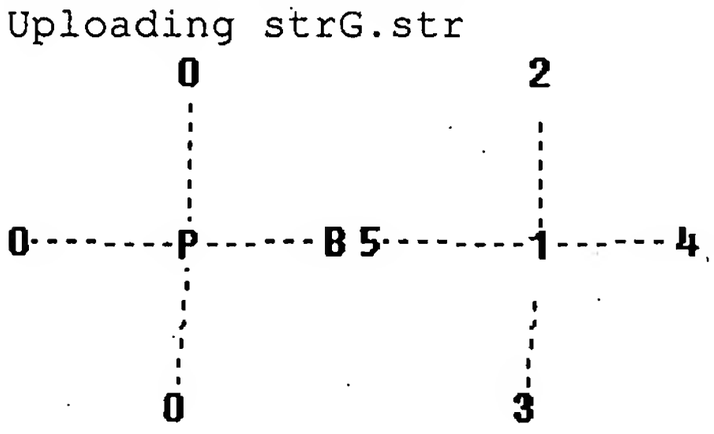


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chain nodes :
1  2  3  4  5
chain bonds :
1-2  1-3  1-4  1-5
exact/norm bonds :
1-2  1-3  1-4  1-5
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Connectivity :
1:4 E exact RC ring/chain  2:1 E exact RC ring/chain  3:1 E exact RC ring/chain
5:1 E exact RC ring/chain
Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS


L3            18 SEA FILE=REGISTRY SSS FUL L1
L4            13 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L5            13 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L4 AND (PRY<=2006 OR AY<=2006
                 OR PY<=2006)
L6          1160 SEA FILE=HCAPLUS ABB=ON  PLU=ON  FISCHER B?/AU
L7             1 SEA FILE=HCAPLUS ABB=ON  PLU=ON  NAUM V?/AU
L8             4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (L6 OR L7) AND L5


=> FILE WPIX
FILE 'WPIX' ENTERED AT 14:24:46 ON 24 AUG 2007
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FILE LAST UPDATED:                    22 AUG 2007   <20070822/UP>
MOST RECENT THOMSON SCIENTIFIC UPDATE:    200754    <200754/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE

>>> Now containing more than 1 million chemical structures in DCR <<<

>>> IPC Reform backfile reclassification has been loaded to 31 May
    2007. No update date (UP) has been created for the reclassified
    documents, but they can be identified by 20060101/UPIC and
    20061231/UPIC and 20060601/UPIC. <<<

>>> Indian patent publication number format enhanced in DWPI - see NEWS <<<

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http://scientific.thomson.com/support/patents/coverage/latestupdates/

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    PLEASE SEE
http://www.stn-international.de/stndatabases/details/dwpi_r.html <<<
'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

=> D QUE L14
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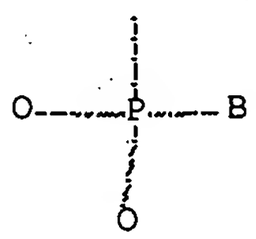


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Structure attributes must be viewed using STN Express query preparation.
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L12           386 SEA FILE=WPIX ABB=ON  PLU=ON  FISCHER B?/AU
L13             1 SEA FILE=WPIX ABB=ON  PLU=ON  NAUM V?/AU
L14             1 SEA FILE=WPIX ABB=ON  PLU=ON  L11 AND (L12 OR L13)


=> DUP REM L14 L8
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PROCESSING COMPLETED FOR L14
PROCESSING COMPLETED FOR L8
L15             4 DUP REM L14 L8 (1 DUPLICATE REMOVED)
                  ANSWER '1' FROM FILE WPIX
                  ANSWERS '2-4' FROM FILE HCAPLUS

=> D IALL ABEQ TECH  HITSTR 1; D IBIB ED ABS HITSTR 2-4

L15  ANSWER 1 OF 4  WPIX COPYRIGHT 2007       THE THOMSON CORP on STN DUPLICATE
     1
ACCESSION NUMBER:      2005-658168 [67]   WPIX
DOC. NO. CPI:          C2005-198714 [67]
TITLE:                 New inorganic boranophosphate salt for use in manufacture
                       of pharmaceutical preparation for boron neutron-capture
                       therapy of cancer, or as synthetic building blocks in
                       synthesis of borano nucleotides
DERWENT CLASS:         B05; B06; D16; D25; E11; E37
INVENTOR:              FISCHER B; NAHUM V; NAUM V
PATENT ASSIGNEE:       (UYBA-N) UNIV BAR-ILAN
COUNTRY COUNT:         106

PATENT INFORMATION:

      PATENT NO       KIND DATE     WEEK     LA  PG          MAIN IPC
      ------------------------------------------------------------------
      WO 2005072062   A2 20050811 (200567)* EN  33[6]       C01B000-00
      US 20070160682  A1 20070712 (200747)  EN

APPLICATION DETAILS:

      PATENT NO       KIND                   APPLICATION    DATE
      ------------------------------------------------------------------
      WO 2005072062 A2                       WO 2005-IL118 20050202
      US 20070160682 A1                      WO 2005-IL118 20050202
      US 20070160682 A1                      US 2006-588074 20060731

PRIORITY APPLN. INFO: US 2004-540343 20040202
INT. PATENT CLASSIF.:
        MAIN:      C01B
   IPC ORIGINAL:   A61K0033-42 [I,A]; A61K0033-42 [I,C]; C01B0035-00 [I,C];
                   C01B0035-10 [I,A]; C07H0019-00 [I,C]; C07H0019-04 [I,A]
BASIC ABSTRACT:
          WO 2005072062 A2   UPAB: 20051223
           NOVELTY - An inorganic boranophosphate salt is new.
           DETAILED DESCRIPTION - Inorganic boranophosphate salt of formula (2) is
     new.
```

M = counterion.

An INDEPENDENT CLAIM is also included for a method for the preparation of inorganic boranophosphate salt (2).

USE - For use in the manufacture of pharmaceutical preparation for boron neutron-capture therapy of cancer, or as synthetic building blocks in the synthesis of borano nucleotides (claimed), as fertilizers, in detergent formulations, or as additive in melts for the glass industry.

ADVANTAGE - The inorganic boranophosphate ion is an excellent mimic of inorganic phosphate. It has high water solubility, acid-base character, and H-bonding properties. MANUAL CODE: CPI: B05-B02A; B05-B02C; B06-H; B07-H; B10-B04; B14-H01;
D05-C; D11-A; E05-T; E06-H; E07-H; E10-B04A1; E10-B04C2; E31-Q08

TECH

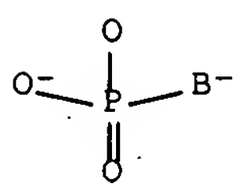
INORGANIC CHEMISTRY - Preparation (claimed): Inorganic boranophosphate salt of formula (2) is prepared by reacting tris(trimethylsilyl)-phosphite with borane-dimethylsulfide complex of formula BH3SMe2, in dry acetonitrile under inert gas, and treating the formed intermediate with a base MOH in water or methanol, to obtain the desired salt.
Preferred Method: The method comprises treating the intermediate with triethylammonium bicarbonate buffer, thus resulting in Et3NH+ salt.
ORGANIC CHEMISTRY - Preparation (claimed): Inorganic boranophosphate salt of formula (2) is prepared by reacting tris(trimethylsilyl)-phosphite with borane-dimethylsulfide complex of formula BH3SMe2, in dry acetonitrile under inert gas, and treating the formed intermediate with a base MOH in water or methanol, to obtain the desired salt.
Preferred Method: The method comprises treating the intermediate with triethylammonium bicarbonate buffer, thus resulting in Et3NH+ salt.
ORGANIC CHEMISTRY - Preferred Components: The base is methanolic ammonia or aqueous ammonium hydroxide solution, thus resulting in the ammonium salt, where M is NH4+.
The base is tributylamine, Bu3N, in methanol, thus resulting in tributylammonium salt, where M is Bu3NH+.

AN.S DCR-1140350
CN.P AMMONIUM BORANOPHOSPHATE
SDCN RAJ710

CM 1

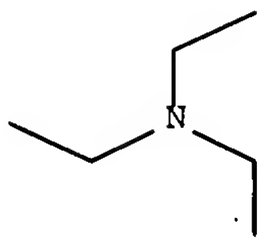
N

CM 2



AN.S DCR-1140351
CN.S TRIETHYLAMMONIUM BORANOPHOSPHATE
SDCN RAJ711

CM 1



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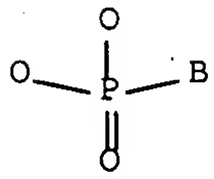

L15 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1342390 HCAPLUS Full-text
DOCUMENT NUMBER: 146:75332
TITLE: Dinucleoside poly(borano)phosphate derivatives and uses thereof
INVENTOR(S): **Fischer, Bilha**; Nahum, Victoria
PATENT ASSIGNEE(S): Bar-Ilan University, Israel
SOURCE: U.S. Pat. Appl. Publ., 19pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2006287271	A1	20061221	US 2006-452244		20060614 <--
PRIORITY APPLN. INFO.:			US 2005-690472P	P	20050615 <--
			US 2005-690475P	P	20050615 <--

OTHER SOURCE(S): MARPAT 146:75332
ED Entered STN: 22 Dec 2006
AB Dinucleoside poly(borano)phosphates are provided that can be useful for prevention or treatment of diseases or disorders modulated by P2Y receptors such as type 2 diabetes, cystic fibrosis and cancer.
IT **848985-86-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(dinucleoside poly(borano)phosphate derivs. and uses thereof for treatment of diseases or disorders modulated by P2Y receptors)
RN 848985-86-4 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, (T-4)-, trihydrogen, compd.

with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

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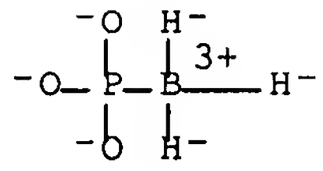
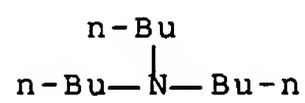
CRN 697244-48-7
CMF B H3 O3 P . 3 H
CCI CCS



3 H^+

CM 2

CRN 102-82-9
CMF C12 H27 N



L15 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:165883 HCAPLUS Full-text
DOCUMENT NUMBER: 144:412817
TITLE: Diadenosine and Diuridine Poly(borano)phosphate Analogs: Synthesis, Chemical and Enzymatic Stability, and Activity at P2Y1 and P2Y2 Receptors
AUTHOR(S): Nahum, Victoria; Tulapurkar, Mohan; Levesque, Sebastien A.; Sevigny, Jean; Reiser, Georg; **Fischer, Bilha**
CORPORATE SOURCE: Department of Chemistry, Gonda-Goldschmied Medical Research Center, Bar-Ilan University, Ramat-Gan, 52900, Israel
SOURCE: Journal of Medicinal Chemistry (**2006**), 49(6), 1980-1990
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 144:412817
ED Entered STN: 23 Feb 2006
AB Dinucleoside polyphosphates, NpnN', exert their physiol. effects via P2 receptors. They are attractive drug targets as they offer better stability and specificity compared to nucleotides, the most common P2-receptor ligands. To further improve the properties of NpnN', which are still pharmacol. unsatisfactory, we developed novel boranophosphate isosteres of dinucleoside

polyphosphates, denoted as Npn(B)N. These analogs were obtained in a facile and efficient synthesis as the exclusive products in a concerted reaction of two nucleoside phosphorimidazolides and inorg. boranophosphate. This unusual reaction is due to the pre-organization of three reactant mols. by the Mg2+ ion. We found that Ap3/5(β/γ-B)A analogs were potent P2Y1-R agonists. Ap5(γ-B)A was equipotent to 2-MeS-ADP (EC50 6.3 + 10-8 M), thus making it one of the most potent P2Y1-R agonists currently known. Moreover, Ap5(γ-B)A did not activate P2Y2-R. In contrast, Up3/5(β/γ-B)U analogs were extremely poor agonists of both P2Y1-R and P2Y2-R. Npn(B)N analogs exhibited remarkable chemical stability under physiol. conditions. Under conditions mimicking gastric juice, Np3(β-B)N analogs exhibited a half-life (t1/2) of 1.3 h, whereas Np5(γ-B)N degraded at a much faster rate (t1/2 18 min). The hydrolysis of Ap3(β-B)A by human nucleotide pyrophosphatase phosphodiesterases (NPP1 and NPP3) was slowed by 40% and 59%, resp., as compared to Ap3A. However, this effect of the boranophosphate was position-dependent, as Np5(γ-B)N was degraded at a rate comparable to that of Np5N. In summary, Ap5(γ-B)A appears to be a highly potent and selective P2Y1-R agonist, as compared to the parent compound This promising scaffold will be applied in the design of future metabolically stable analogs.

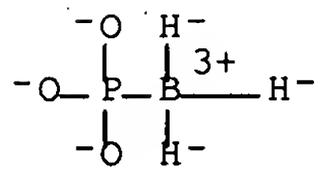
IT 848985-86-4
RL: RGT (Reagent); RACT (Reactant or reagent)
(synthesis, chemical and enzymic stability, and activity at P2Y1 and P2Y2 receptors)

RN 848985-86-4 HCAPLUS

CN Borate(3-), trihydro[phosphito(3-)-κP]-, (T-4)-, trihydrogen, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

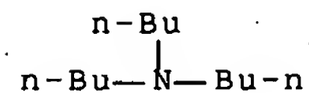
CRN 697244-48-7
CMF B H3 O3 P . 3 H
CCI CCS



3 H+

CM 2

CRN 102-82-9
CMF C12 H27 N



REFERENCE COUNT: 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L15 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:928329 HCAPLUS Full-text
DOCUMENT NUMBER: 142:366086
TITLE: Boranophosphate salts as an excellent mimic of phosphate salts: Preparation, characterization, and properties
AUTHOR(S): Nahum, Victoria; **Fischer, Bilha**
CORPORATE SOURCE: Department of Chemistry, Gonda-Goldschmied Medical Research Center, Bar-Ilan University, Ramat-Gan, 52900, Israel
SOURCE: European Journal of Inorganic Chemistry (**2004**), (20), 4124-4131
CODEN: EJICFO; ISSN: 1434-1948
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 04 Nov 2004
AB The authors report on the preparation of boranophosphate salts, BPi (2), and the exploration of their properties with a view to developing a new mimic of the parent phosphate. BPi salts were easily prepared in excellent yield in a 1-pot two-step reaction from tris(trimethylsilyl) phosphite, and were characterized by x-ray crystallog. and IR, 1H and 31P NMR spectroscopy. The authors evaluated the acid/base character of BPi by determining its acidity consts. Likewise, the authors evaluated the stability of BPi at various pH values, and calculated the decomposition-rate consts. at highly acidic pH. The authors also monitored the H-bonded clustering of BPi in organic solvents, including MeOH. Finally, the authors explored the chemical behavior of BPi with respect to various organic and inorg. reagents. BPi is stable under the following conditions: both basic and acidic pH (pH > 2), in the presence of amines, and in the presence of Mg2+ ions. However, a P-B bond cleavage is observed upon the reaction of BPi with carbodiimides or upon catalytic hydrogenation. The reducing nature of the BH3 moiety is drastically decreased in BPi. Likewise, the nucleophilicity of BPi's O atom is lower than in phosphate, Pi, salts. Based on its water solubility, acid-base character, and H-bonding properties, BPi appears as a perfect mimic of Pi and is an attractive alternative to the known phosphate isosters.
IT **848985-87-5**
RL: PRP (Properties)
(IR spectrum of)
RN 848985-87-5 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, (T-4)-, trihydrogen, compd. with N,N-diethylethanamine (1:2) (9CI) (CA INDEX NAME)

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CRN 697244-48-7
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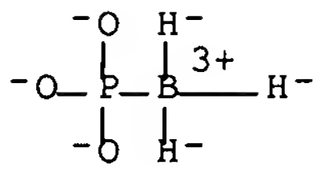
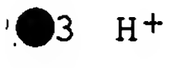
CCI CCS





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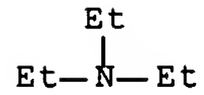
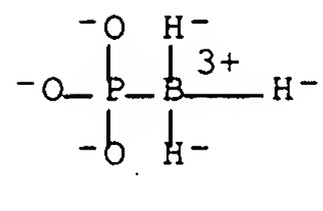
CMF C6 H15 N



IT **848985-86-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and hydrogen bonding in organic solvents)
RN 848985-86-4 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, (T-4)-, trihydrogen, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

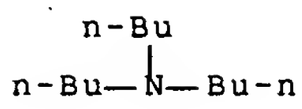
CM 1

CRN 697244-48-7
CMF B H3 O3 P . 3 H
CCI CCS



CM 2

CRN 102-82-9
CMF C12 H27 N



IT **848985-88-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 848985-88-6 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, hydrogen (T-4)-trihydro[phosphito(3-)-κP]borate(3-) (2:1:1) (9CI) (CA INDEX NAME)

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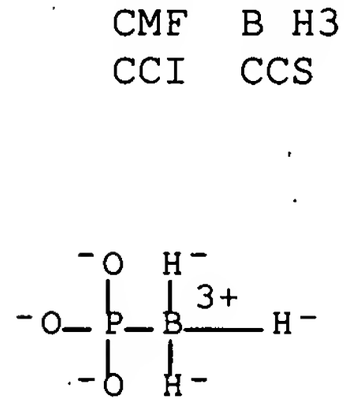
CRN 178449-22-4
CMF B H3 O3 P
CCI CCS



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CRN 10549-76-5
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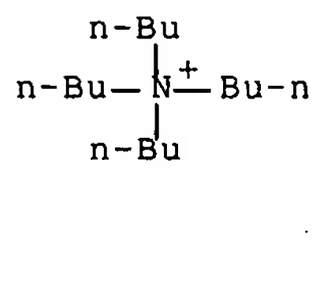
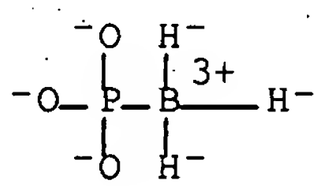
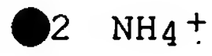


IT **848985-85-3P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure, hydrogen bonding in organic solvents, acid-base properties, and chemical reactivity)
RN 848985-85-3 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, diammonium hydrogen, (T-4)-(9CI) (CA INDEX NAME)





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L1                STR
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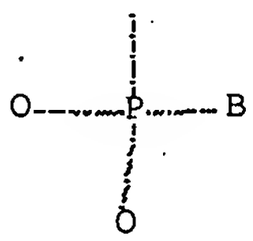


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L4            13 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L3
L5            13 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L4 AND (PRY<=2006 OR AY<=2006
                 OR PY<=2006)


=> S L5 NOT L8
L16           9 L5 NOT L8

=> FILE WPIX
FILE 'WPIX' ENTERED AT 14:25:52 ON 24 AUG 2007
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http://scientific.thomson.com/support/patents/coverage/latestupdates/

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http://www.stn-international.de/stndatabases/details/dwpi_r.html <<<
'BI,ABEX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

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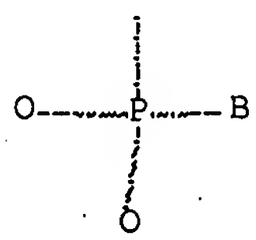

Structure attributes must be viewed using STN Express query preparation.
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L11 1 SEA FILE=WPIX ABB=ON PLU=ON L10/DCR

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L17 0 L11 NOT L14

=> DUP REM L17 L16
L17 HAS NO ANSWERS
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FILE COVERS 1907 - 24 Aug 2007 VOL 147 ISS 10

FILE LAST UPDATED: 23 Aug 2007 (20070823/ED)

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PROCESSING COMPLETED FOR L17
PROCESSING COMPLETED FOR L16
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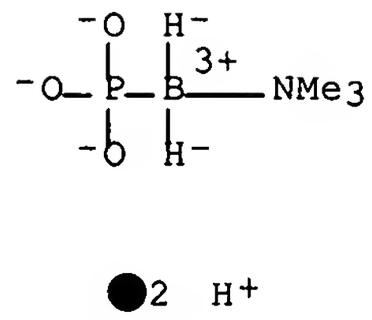
ANSWERS '1-9' FROM FILE HCAPLUS

=> D IBIB ED ABS HITSTR 1-9

L18 ANSWER 1 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:638056 HCAPLUS Full-text
DOCUMENT NUMBER: 145:261858
TITLE: Lewis base stabilized phosphanylborane
AUTHOR(S): Schwan, Karl-Christian; Timoskin, Alexey Y.; Zabel, Manfred; Scheer, Manfred
CORPORATE SOURCE: Institut fuer Anorganische Chemie der Universitaet Regensburg, Regensburg, 93040, Germany
SOURCE: Chemistry--A European Journal (2006), 12(18), 4900-4908
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 145:261858
ED Entered STN: 02 Jul 2006
AB The abstraction of the Lewis acid from [W(CO)5(PH2BH2·NMe3)] (1) by an excess of P(OMe3)3 leads to the quant. formation of the first Lewis base stabilized monomeric parent compound of phosphanylborane [H2PBH2·NMe3] (2). D. functional theory (DFT) calcns. showed a low energetic difference between the crystallog. determined antiperiplanar arrangement of the lone pair and the trimethylamine group relative to the P-B core and the synperiplanar conformation. Subsequent reactions with the main-group Lewis acid BH3 as well as with an [Fe(CO)4] unit as a transition-metal Lewis acid gave [(BH3)PH2BH2·NMe3] (3), containing a central H3B-PH2-BH2 unit, and [Fe(CO)4(PH2BH2·NMe3)] (4), resp. In oxidation processes with O2, Me3NO, elemental sulfur, and selenium, the boranylphosphine chalcogenides [H2P(Q)BH2·NMe3] (Q = S 5b; Se 5c) as well as the novel boranylphosphonic acid [(HO)2P(O)BH2·NMe3] (6a) are formed. All products were characterized by spectroscopic as well as by single-crystal x-ray structure anal.
IT **905911-76-4P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure)
RN 905911-76-4 HCAPLUS
CN Borate(2-), (N,N-dimethylmethanamine)dihydro[phosphito(3-)-κP]-, dihydrogen, (T-4)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 2 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:430908 HCAPLUS Full-text
DOCUMENT NUMBER: 141:17622
TITLE: Preparation of 2'-fluoro substituted oligoribonucleotides and compositions for use in treatment of obesity and diabetes
INVENTOR(S): Allerson, Charles; Bhat, Balkrishen; Eldrup, Anne B.; Manoharan, Muthiah; Griffey, Richard H.; Baker, Brenda F.; Swayze, Eric E.
PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., USA
SOURCE: PCT Int. Appl., 149 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 46
PATENT INFORMATION:

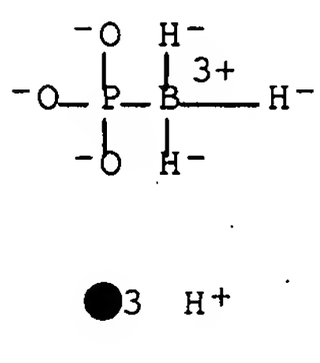
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004044136	A2	20040527	WO 2003-US35071	20031104 <--
WO 2004044136	A3	20050224		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2504929	A1	20040527	CA 2003-2504929	20031104 <--
AU 2003287502	A1	20040603	AU 2003-287502	20031104 <--
EP 1560840	A2	20050810	EP 2003-781743	20031104 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.:
US 2002-423760P P 20021105 <--
WO 2003-US35071 W 20031104 <--

ED Entered STN: 27 May 2004

AB The present invention provides methods for preparation of 2'-fluoro substituted oligoribonucleotides and compns. for use in treatment of obesity and diabetes. The compns. are useful for targeting selected nucleic acid mols. and modulating the expression of one or more genes. In preferred embodiments the compns. of the present invention hybridize to a portion of a target RNA resulting in loss of normal function of the target RNA.

IT 697244-48-7
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(phosphodiester internucleoside linking group; preparation of 2'-fluoro substituted oligoribonucleotides and compns. for use in treatment of obesity and diabetes)
RN 697244-48-7 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, trihydrogen, (T-4)- (9CI) (CA INDEX NAME)



3 H+

L18 ANSWER 3 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:414675 HCAPLUS Full-text
DOCUMENT NUMBER: 140:405475
TITLE: Modulation of immunostimulatory properties of oligonucleotide-based compounds by optimal presentation of 5' ends
INVENTOR(S): Agrawal, Sudhir; Kandimalla, Ekambar R.; Yu, Dong; Bhagat, Lakshmi
PATENT ASSIGNEE(S): Hybridon, Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 67 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
US 2004097719	A1	20040520	US 2002-279684		20021024 <--
US 2006019909	A1	20060126	US 2004-925872		20040825 <--
US 2007173469	A1	20070726	US 2004-925873		20040825 <--
US 2006287262	A1	20061221	US 2005-174450		20050701 <--
PRIORITY APPLN. INFO.:			US 2001-344767P	P	20011024 <--
			US 2002-376623P	P	20020430 <--
			US 2002-399181P	P	20020729 <--
			US 2002-399287P	P	20020729 <--
			US 2002-399302P	P	20020729 <--
			US 2002-399343P	P	20020729 <--
			US 2002-399344P	P	20020729 <--
			US 2002-279684	A3	20021024 <--

OTHER SOURCE(S): MARPAT 140:405475
ED Entered STN: 21 May 2004
AB The authors disclose the therapeutic use of oligonucleotides as immunostimulatory agents in immunotherapy applications. More particularly, the invention provides linear and branched oligonucleotides joined by their 3'-terminus (immunomers) for generating an immune response or for treating a

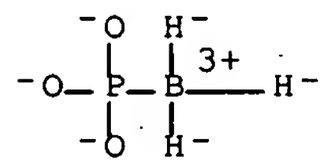
patient in need of immunostimulation. The immunomers of the invention comprise at least two oligonucleotides linked at their 3' ends, internucleoside linkages or functionalized nucleobase or sugar to a non-nucleotidic linker, at least one of the oligonucleotides being an immunostimulatory oligonucleotide and having an accessible 5' end.

IT **178449-22-4**

RL: BSU (Biological study, unclassified); BIOL (Biological study) (as linker for linear and branched immunostimulatory oligonucleotides joined by their 3'-terminus)

RN 178449-22-4 HCAPLUS

CN Borate(3-), trihydro[phosphito(3-)-κP]-, (T-4)- (9CI) (CA INDEX NAME)



L18 ANSWER 4 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:937534 HCAPLUS Full-text

DOCUMENT NUMBER: 140:121429

TITLE: (C6H14N2){Zn[ZnB2P4O15(OH)2]·(C6H13N2)Cl}: A New Templated Zincoborophosphate

AUTHOR(S): Huang, Ya-Xi; Schaefer, Gerd; Carrillo-Cabrera, Wilder; Borrmann, Horst; Gil, Raul Cardoso; Kniep, Ruediger

CORPORATE SOURCE: Max-Planck-Institut fuer Chemische Physik fester Stoffe, Dresden, D-01187, Germany

SOURCE: Chemistry of Materials (2003), 15(26), 4930-4935
CODEN: CMATEX; ISSN: 0897-4756

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

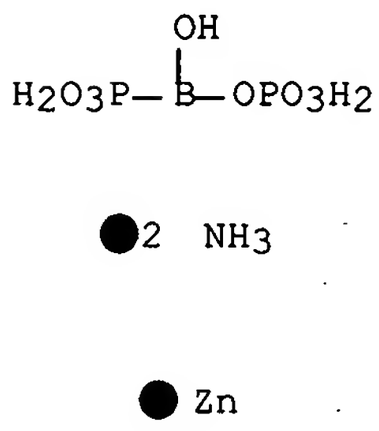
ED Entered STN: 02 Dec 2003

AB Colorless crystals of (C6H14N2){Zn[ZnB2P4O15(OH)2]·(C6H13N2)Cl} (1) were prepared from mixts. of ZnCl2, B2O3, diazabicyclo[2.2.2]octane (DABCO), and 85% H3PO4 under mild hydrothermal conditions (170°). The crystal structure was determined by single-crystal x-ray diffraction (monoclinic, space group P21/c, a 1704.3(1), b 937.03(5), c 1619.75(8) pm, β 96.894(3)°, Z = 2). The crystal structure contains tetrahedral zigzag ribbons, 1∞{[ZnB2P4O15(OH)2]4-}, running along [010]. Addnl. ZnO2NCl tetrahedra at the borders complete the ribbons by sharing common O-corners with the zincoborophosphate polymer. The N atoms of the quaternary ZnO2NCl tetrahedra belong to monoprotonated (HDABCO)+ ions. A 2nd (diprotonated) species, (H2DABCO)2+, acts as a pure template and is fixed to adjacent zincoborophosphate ribbons along [100] via H bonds. The title compound 1 can be described as an adduct of (C6H14N2){Zn[ZnB2P4O15(OH)2]} with diazabicyclo[2.2.2]octane- hydrochloride. Thermoanal. and x-ray powder diffraction studies to high temps. (740°) show the decomposition of 1 and the formation of a NH4[ZnBP2O8] polymorph as an intermediate.

IT **648416-69-7**

RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative) (formation in thermal decomposition of zincoborophosphate with DABCO)

RN 648416-69-7 HCAPLUS
CN Phosphoric acid, B-monoanhydride with boronophosphonic acid, ammonium zinc salt (1:2:1) (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 5 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2004:256208 HCAPLUS Full-text
DOCUMENT NUMBER: 140:400753
TITLE: Reading, writing, and modulating genetic information with boranophosphate mimics of nucleotides, DNA, and RNA
AUTHOR(S): Shaw, Barbara Ramsay; Dobrikov, Mikhail; Wang, Xin; Wan, Jing; He, Kaizhang; Lin, Jin-Lai; Li, Ping; Rait, Vladimir; Sergueeva, Zinaida A.; Sergueev, Dmitri
CORPORATE SOURCE: Paul M. Gross Chemical Laboratory, Department of Chemistry, Duke University, Durham, NC, 27708-0346, USA
SOURCE: Annals of the New York Academy of Sciences (2003), 1002(Therapeutic Oligonucleotides), 12-29
CODEN: ANYAA9; ISSN: 0077-8923
PUBLISHER: New York Academy of Sciences
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
ED Entered STN: 29 Mar 2004

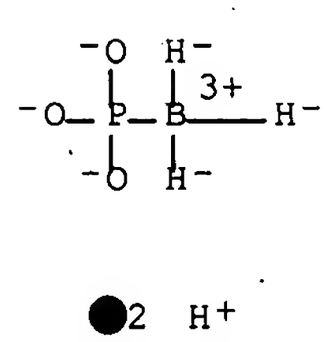
AB A review. The P-boranophosphates are efficient and near perfect mimics of natural nucleic acids in permitting reading and writing of genetic information with high yield and accuracy. Substitution of a borane (-BH3) group for oxygen in the phosphate ester bond creates an isoelectronic and isosteric mimic of natural nucleotide phosphate esters found in mononucleotides, i.e., AMP and ATP, and in RNA and DNA polynucleotides. Compared to natural nucleic acids, the boranophosphate RNA and DNA analogs demonstrate increased lipophilicity and resistance to endo- and exonucleases, yet they retain neg. charge and similar spatial geometry. Borane groups can readily be introduced into the NTP and dNTP nucleic acid monomer precursors to produce α-P-borano nucleoside triphosphate analogs (e.g., NTPαB and dNTPαB). The NTPαB and dNTPαB are, in fact, good to excellent substrates for RNA and DNA polymerases, resp., and allow ready enzymic synthesis of RNA and DNA with P-boranophosphate linkages. Further, boranophosphate polymer products are good templates for replication, transcription, and gene expression; boronated RNA products are also suitable for reverse transcription to cDNA. Fully substituted boranophosphate DNA can activate the RNase H cleavage of RNA in RNA-DNA hybrids. Moreover, certain dideoxy-NTPαB analogs appear to be better

substrates for viral reverse transcriptases than the regular ddNTPs, and may offer promising prodrug alternatives in antiviral therapy. These properties make boranophosphates promising candidates for diagnostics; aptamer selection; gene therapy; and antiviral, antisense, and RNAi therapeutics. The boranophosphates constitute a versatile family of phosphate mimics for processing genetic information and modulating gene function.

IT **148099-10-9**
RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)
(modulating genetic information with boranophosphate mimics of nucleotides, DNA and RNA)

RN 148099-10-9 HCAPLUS

CN Borate(3-), trihydro[phosphito(3-)-κP]-, dihydrogen, (T-4)- (9CI) (CA INDEX NAME)



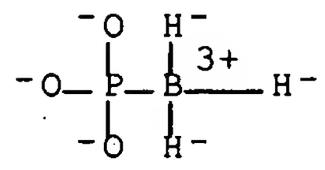
REFERENCE COUNT: 89 THERE ARE 89 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L18 ANSWER 6 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1996:379885 HCAPLUS Full-text
DOCUMENT NUMBER: 125:87085
TITLE: Hydrolysis of Thymidine Boranomonophosphate and Stepwise Deuterium Substitution of the Borane Hydrogens. 31P and 11B NMR Studies
AUTHOR(S): Li, Hong; Hardin, Charles; Shaw, Barbara Ramsay
CORPORATE SOURCE: Department of Chemistry, Duke University, Durham, NC, 27708, USA
SOURCE: Journal of the American Chemical Society (1996), 118(28), 6606-6614
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 02 Jul 1996

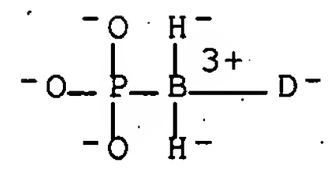
AB The α-P-boranophosphate nucleosides comprise a new class of modified nucleotides that may find use as therapeutic and DNA diagnostic agents. Hydrolysis of thymidine 5'-boranomonophosphate, d(pBT), has been studied in H2O and D2O using 1H, 31P, and 11B NMR spectroscopies. Although d(pBT) is quite stable at 25 °C, it hydrolyzes slowly at higher temps. At 50 or 60 °C, d(pBT) hydrolyzes first into thymidine (dT) and boranophosphate (O3P-BH33-), followed by subsequent hydrolysis of the O3P-BH33- to produce phosphonate and boric acid. A three-step deuterium substitution of the borane hydrogens in O3P-BH33- was detected in D2O by the presence of a 31P isotope shift. The 31P resonances shifted downfield by 0.14 ppm upon substitution of each of three 1H atoms by 2H. Exchange of the borane hydrogens with D2O occurs as sequential processes superimposed upon hydrolysis of O3P-BH33-. The hydrolysis and deuteration steps were characterized in terms of pseudo-first-order rate

consts. Hydrolysis of O3P-BH33- is about 10-fold slower than deuterium substitution.

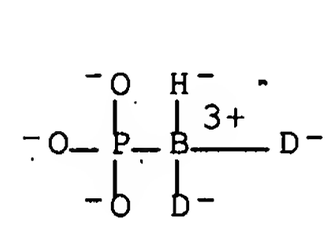
IT **178449-22-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(hydrolysis of thymidine boranomonophosphate and stepwise deuterium substitution of the borane hydrogens)
RN 178449-22-4 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, (T-4)- (9CI) (CA INDEX NAME)



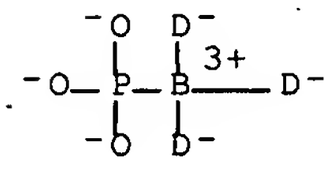
IT **178449-24-6P 178449-25-7P 178449-26-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(hydrolysis of thymidine boranomonophosphate and stepwise deuterium substitution of the borane hydrogens)
RN 178449-24-6 HCAPLUS
CN Borate(3-), trihydro-d-[phosphito(3-)-P]-, (T-4)- (9CI) (CA INDEX NAME)



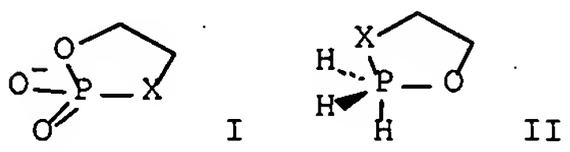
RN 178449-25-7 HCAPLUS
CN Borate(3-), trihydro-d2-[phosphito(3-)-P]-, (T-4)- (9CI) (CA INDEX NAME)



RN 178449-26-8 HCAPLUS
CN Borate(3-), trihydro-d3-[phosphito(3-)-P]-, (T-4)- (9CI) (CA INDEX NAME)



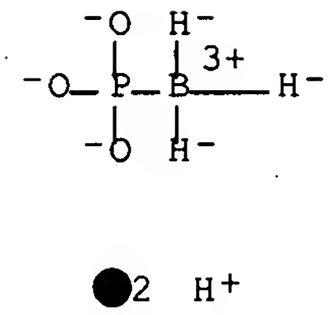
L18 ANSWER 7 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1993:408879 HCAPLUS Full-text
DOCUMENT NUMBER: 119:8879
TITLE: Phosphonates as mimics of phosphate biomolecules: ab initio calculations on tetrahedral ground states and pentacoordinate intermediates for phosphoryl transfer
AUTHOR(S): Thatcher, Gregory R. J.; Campbell, A. Stewart
CORPORATE SOURCE: Dep. Chem., Queen's Univ., Kingston, ON, K7L 3N6, Can.
SOURCE: Journal of Organic Chemistry (1993), 58(8), 2272-81
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
ED Entered STN: 10 Jul 1993
GI



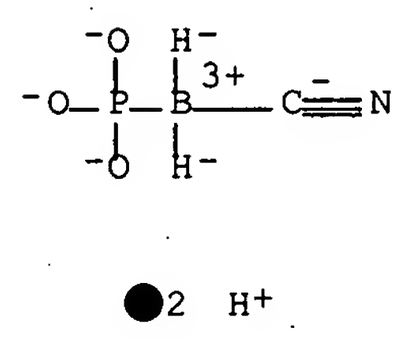
I II

AB The use of phosphonates as analogs of phosphate biomols. was explored using ab initio SCF calcns. at the 3-21+G(*) levels. Fully optimized geometries were obtained for the tetrahedral ground-state monoanions CHF2PO3H-, CH2FPO3H-, CH3PO3H-, BH3PO3H2-, H2PO3-, and I (X = O, CFH) and torsional energy profiles obtained for CH2FPO3H- and H2PO3. Comparison was made of (1) structure and conformational dependence for these species and (2) electrostatic potential maps for ethylene phosphate and its (monofluoromethylene)phosphonate analog. The results suggest that, despite the isopolar relationship of (fluoromethyl)phosphonates and the parent phosphates, binding at a receptor site may be considerably perturbed for the phosphonate analogs. Fully optimized geometries were located for isomers of the pentacoordinate trigonal bipyramidal species PH4X (X = CH3, CF3, CF2H, CFH2, BH3-, BF3-, O-, OH) and II (X = O, CH2, CFH, CF2). Torsional energy profiles were explored for PH4X (X = CH3, CF3, CF2H, CFH2). The calculated relative apicophilicity scale in PH4X (CF3 > CF2H > CFH2 > CH3 > OH > O- ≥ BF3- > BH3-) varies in the five-membered cyclic phosphoranes II only by reversal of CH3 and OH. It is concluded that (mono- and difluoromethylene)phosphonates have similar ligand preferences to the parent phosphates in the pentacoordinate state. These phosphonates are capable of forming transition-state analogs at the active site of phosphoryl transfer enzymes.

IT **148099-10-9**
RL: PRP (Properties)
(MO calcns. and conformation of)
RN 148099-10-9 HCAPLUS
CN Borate(3-), trihydro[phosphito(3-)-κP]-, dihydrogen, (T-4)- (9CI) (CA INDEX NAME)



L18 ANSWER 8 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1991:680124 HCAPLUS Full-text
DOCUMENT NUMBER: 115:280124
TITLE: Boron analogs of phosphonoacetates: synthesis, characterization and antitumor properties of sodium diethyl phosphite-carboxyborane and related compounds
AUTHOR(S): Sood, Anup; Sood, Cynthia K.; Hall, Iris H.; Spielvogel, B. F.
CORPORATE SOURCE: P. M. Gross Chem. Lab., Duke Univ., Durham, NC, 27706, USA
SOURCE: Tetrahedron (1991), 47(34), 6915-30
CODEN: TETRAB; ISSN: 0040-4020
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 115:280124
ED Entered STN: 27 Dec 1991
AB Several methods were investigated for the synthesis of functionalized phosphite-borane adducts. The monosodium salt of diethylphosphite-carboxyborane (a B analog of Na diethylphosphonoacetate) and related precursors and derivs. were prepared A brief description of their cytotoxic and antitumor properties is also presented.
IT **137484-31-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and cytotoxic activity of)
RN 137484-31-2 HCAPLUS
CN Borate(3-), (cyano-C)dihydro[phosphito(3-)-P]-, trihydrogen, (T-4)- (9CI) (CA INDEX NAME)



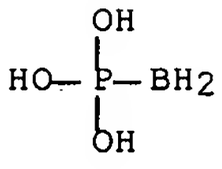
L18 ANSWER 9 OF 9 HCAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 1989:594820 HCAPLUS Full-text
DOCUMENT NUMBER: 111:194820
TITLE: Homolytic reactions of ligated boranes. Part 10. Electron spin resonance studies of radicals derived from ligated arylboranes

AUTHOR(S): Paul, Vikram; Roberts, Brian P.
CORPORATE SOURCE: Christopher Ingold Lab., Univ. Coll. London, London, WC1H 0AJ, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1988), (10), 1895-901
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:194820
ED Entered STN: 25 Nov 1989

AB The ligated arylboryl radicals L→B•HR [L = Me3N, Et3P, (MeO)3P; R = Ph, 4-Me3CC6H4] were generated in oxirane solvent by hydrogen atom abstraction from L→BH2R using tert-butoxyl radicals produced by UV photolysis of di-tert-Bu peroxide. The ESR spectra of the phosphine- or phosphite-ligated radicals show that there is substantial conjugative delocalization of the unpaired electron from B onto the aromatic rings, although this delocalization is less extensive than in comparable benzylic carbon-centered radicals. The results of ab initio MO calcns. support the proposal that hyperconjugative delocalization onto the P ligand completes with conjugative delocalization onto the ring in the complexed arylboryl radicals. The ESR spectra of the amine-arylboryl radicals were too weak to detect, although these radicals and Et3P→B•HR abstract halogen atoms readily from alkyl bromides to afford spectra of the corresponding alkyl radicals. The ligated arylboryl radicals are less reactive and more selective in bromine atom abstraction than homoleptic ligated alkylboryl radicals, presumably because the former are appreciably stabilized by conjugative delocalization of the unpaired electron onto the aromatic rings.

IT **123324-74-3**
RL: PROC (Process)
(ab initio MO calcn. of)

RN 123324-74-3 HCAPLUS
CN Phosphoranyl, boryltrihydroxy- (9CI) (CA INDEX NAME)



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L3           18 SEA SSS FUL L1

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L4           13 SEA ABB=ON  PLU=ON  L3
L5           13 SEA ABB=ON  PLU=ON  L4 AND (PRY<=2006 OR AY<=2006 OR PY<=2006)

L6         1160 SEA ABB=ON  PLU=ON  FISCHER B?/AU
L7            1 SEA ABB=ON  PLU=ON  NAUM V?/AU
L8            4 SEA ABB=ON  PLU=ON  (L6 OR L7) AND L5

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L10           3 SEA SSS FUL L1
L11           1 SEA ABB=ON  PLU=ON  L10/DCR
L12         386 SEA ABB=ON  PLU=ON  FISCHER B?/AU
L13           1 SEA ABB=ON  PLU=ON  NAUM V?/AU
L14           1 SEA ABB=ON  PLU=ON  L11 AND (L12 OR L13)

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                D QUE L11
L17           0 SEA ABB=ON  PLU=ON  L11 NOT L14

     FILE 'HCAPLUS' ENTERED AT 14:26:15 ON 24 AUG 2007
L18           9 DUP REM L17 L16 (0 DUPLICATES REMOVED)

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